

Famotidine
76824-35-6 | DTXSID5023039

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.91e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.20e-01

Confidence level: 8.58e-01

Nearest Neighbors from the Training Set

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11

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(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11

Image not found

Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12

Image not found

Myrcene

Measured: 2.15e-10

Predicted: 2.05e-10